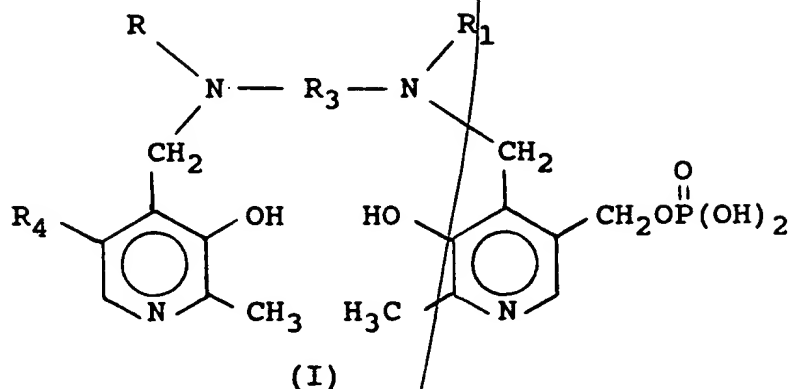


WE CLAIM:

1. A chelating compound of the formula:



wherein

R is hydrogen or



R<sub>1</sub> is hydrogen or



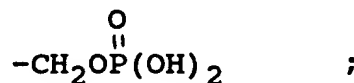
and one of R and R<sub>1</sub> is other than hydrogen;

R<sub>3</sub> is alkylene having from 1 to 8 carbons,

1,2-cycloalkylene having from 5 to 8 carbons,

or 1,2-arylene having from 6 to 10 carbons, or

R<sub>4</sub> is hydrogen, hydroxymethyl, alkyl having from 1 to 6 carbons or



R<sub>5</sub> and R<sub>6</sub> are each, individually, hydroxy,

alkoxy having from 1 to 18 carbons,

hydroxy-substituted alkoxy having from 1 to 18

carbons, amino or alkylamido having from 1 to

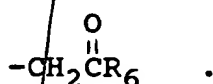
18 carbons;

16 the phosphate group mono and diesters of the  
17 compounds thereof with monohydric and polyhydric  
18 alcohols having from 1 to 18 carbons, or alkylamino  
19 alcohols, each having from 1 to 18 carbons, and  
20 the salts thereof.

1 2. A <sup>chelate</sup>~~chelating~~ compound of Claim 1 wherein R is



2 and R<sub>1</sub> is



1 3. A <sup>chelate</sup>~~chelating~~ compound of Claim 2 wherein R<sub>5</sub> and R<sub>6</sub>  
2 are each, individually, hydroxy, alkoxy having from 1  
3 to 8 carbons, amino or alkylamido having from 1 to 8  
4 carbons.

1 4. A <sup>chelate</sup>~~chelating~~ compound of Claim 3 wherein R<sub>5</sub> and R<sub>6</sub>  
2 are hydroxy or a salt thereof.

1 5. As a <sup>chelate</sup>~~chelating~~ compound of Claim 4,  
2 N,N'-bis-(pyridoxal-5-phosphate)ethylenediamine-  
3 N,N'-diacetic acid or a salt thereof.

1 6. A <sup>chelate</sup>~~chelating~~ compound of Claim 1 wherein R<sub>3</sub> is  
2 alkylene having from 2 to 6 carbons.

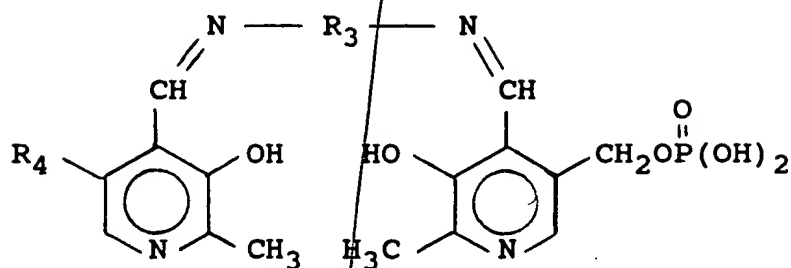
1 7. A <sup>chelate</sup>~~chelating~~ compound of Claim 1 wherein R<sub>3</sub> is  
2 cyclohexyl.

1 8. As a <sup>chelate</sup>~~chelating~~ compound of Claim 7,  
2 N,N'-bis-(pyridoxal-5-phosphate)-trans-1,2-cyclohexyl-  
3 diamine-N,N'-diacetic acid or a salt thereof.

Sub A' 1 9. A <sup>chelate</sup>~~chelating~~ compound of Claim 1, 2, 3, 4, 5, 6, 7,  
2 or 8 with a metal ion having an atomic number within  
3 the range of 21 to 29, 42, 44 or 58-70.

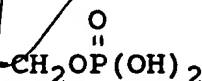
- 1 10. A chelate of Claim 9 wherein the metal ion is  
2 selected from the group consisting of chromium(III),  
3 manganese(II), iron(III), iron(II), cobalt(II),  
4 nickel(II), copper(II), praseodymium(III),  
5 neodymium(III), samarium(III), ytterbium(III),  
6 gadolinium(III), terbium(III), dysprosium(III),  
7 holmium(III) and erbium(III).
- 1 11. A calcium salt of a chelate of Claim 9.
- 1 12. A calcium salt of Claim 11 wherein the molar ratio  
2 of calcium to chelating compound is from 0.05 to  
3 1.0.
- 1 13. A calcium salt of Claim 12 wherein the molar ratio  
2 of calcium to chelating compound is from 0.1 to 0.5.
- Sub A<sup>2</sup> 1 14. A chelate of a compound of Claim 1, 2, 3, 4, 5, 6,  
2 7, or 8 with a manganese(II) ion.
- 1 15. As a chelate of Claim 14, a manganese(II) chelate of  
2 N,N'-bis-(pyridoxal-5-phosphate)ethylenediamine-  
3 N,N'-diacetic acid or a salt thereof.
- 1 16. A calcium salt of the chelate of Claim 15.
- 1 17. A calcium salt of Claim 16 wherein the molar ratio  
2 of calcium to chelating compound is from 0.05 to  
3 1.0.
- 1 18. A calcium salt of Claim 17 wherein the molar ratio  
2 of calcium to chelating compound is from 0.1 to 0.5.
- 1 19. As a chelate of Claim 14, a manganese(II) chelate of  
2 N,N'-bis-(pyridoxal-5-phosphate)-trans-1,2-cyclohexyl  
3 diamine-N,N'-diacetic acid or a salt thereof.

1 20. A chelating compound intermediate of the formula



2 wherein

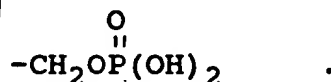
3  $R_3$  is alkylene having from 1 to 8 carbons or  
4 cycloalkyl having from 3 to 8 carbons;  
5  $R_4$  is hydrogen, hydroxyalkyl having from 1 to 6  
6 carbons, alkyl having from 1 to 6 carbons or



7 and the salts thereof.

1 21. A chelating compound intermediate of Claim 20

2 wherein  $R_4$  is



1 22. A chelating compound intermediate of Claim 21

2 wherein  $R_3$  is an alkylene group having from 2 to 6  
3 carbons.

1 23. A chelating compound intermediate of Claim 22

2 wherein  $R_3$  is ethylene.

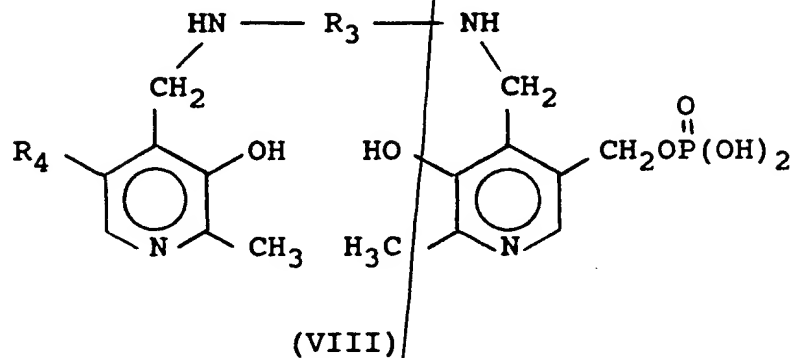
1 24. A chelating compound intermediate of Claim 21

2 wherein  $R_3$  is 1,2-cycloalkylene.

1 25. A chelating compound intermediate of Claim 24

2 wherein  $R_3$  is 1,2-cyclohexyl.

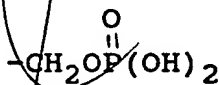
1 26. A chelating compound intermediate of the formula



2 wherein

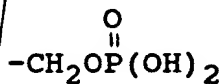
3  $R_3$  is alkylene having from 1 to 8 carbons or  
4 cycloalkyl having from 3 to 8 carbons;

5  $R_4$  is hydrogen, hydroxyalkyl having from 1 to 6  
6 carbons, alkyl having from 1 to 6 carbons or



7 and the salts thereof.

1 27. A chelating compound intermediate of Claim 26  
2 wherein  $R_4$  is



3 and the salts thereof.

1 28. A chelating compound intermediate of Claim 26  
2 wherein  $R_3$  is an alkylene group having from 2 to 6  
3 carbons.

1 29. A chelating compound intermediate of Claim 28  
2 wherein  $R_3$  is ethylene.

1 30. A chelating compound intermediate of Claim 26  
2 wherein  $R_3$  is 1,2-cycloalkylene.

1 31. A chelating compound intermediate of Claim 30  
2 wherein R<sub>3</sub> is 1,2-cyclohexane.

Sub A<sup>3</sup>  
1 32. A NMRI contrast medium composition consisting  
2 essentially of a chelate of a compound of Claim 1,  
3 2, 3, 4, 5, 6, 7 or 8 with a metal ion having an  
4 atomic number of from 21-29, 42, 44 or 58-70 and a  
5 pharmaceutically acceptable, compatible excipient.

1 33. A NMRI contrast medium composition of Claim 32  
2 wherein the metal ion is selected from the group  
3 consisting of chromium(III), manganese(II),  
4 iron(III), iron(II), cobalt(II), nickel(II),  
5 copper(II), praseodymium(III), neodymium(III),  
6 samarium(III), ytterbium(III), gadolinium(III),  
7 terbium(III), dysprosium(III), holmium(III) and  
8 erbium(III).

1 34. An NMRI contrast medium composition of Claim 33  
2 containing a calcium salt of the chelate.

Sub B<sup>8</sup>  
1 35. An NMRI contrast medium composition of Claim 34  
2 containing containing a calcium salt of the chelate  
3 wherein the molar ratio of calcium to chelating  
4 compound is from 0.05 to 1.0.

1 36. An NMRI contrast medium composition of Claim 35  
2 containing a calcium salt wherein the molar ratio of  
3 calcium to chelating compound is from 0.1 to 0.5.

1 37. An NMRI contrast medium composition of Claim 33  
2 wherein the metal ion is manganese(II) ion.

1 38. An NMRI contrast medium composition of Claim 33  
2 wherein the compound is N,N'-bis-(pyridoxal-  
3 5-phosphate)ethylenediamine-N,N'-diacetic acid,  
4 N,N'-bis-(pyridoxal-5-phosphate)-trans-1,2-cyclohexyl  
5 diamine-N,N'-diacetic acid, or a salt thereof.

1 39. An NMRI contrast medium composition of Claim 38  
2 containing a calcium salt.

- 1 40. An NMRI contrast medium composition of Claim 39  
2 containing a calcium salt, wherein the molar ratio  
3 of calcium to chelating compound is from 0.05 to  
4 1.0.
- 1 41. An NMRI contrast medium composition of Claim 40  
2 containing a calcium salt, wherein the molar ratio  
3 of calcium to chelating compound is from 0.1 to 0.5.
- 1 42. An NMRI contrast medium composition of Claim 33  
2 wherein the concentration of chelate salt in the  
3 medium is from 0.001 to 5.0 moles per liter.
- 1 43. An NMRI contrast medium composition of Claim 42  
2 wherein the concentration of chelate salt in the  
3 medium is from 0.1 to 0.5 moles per liter.
- Sub A<sup>4</sup>  
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AU. 335
- 2 44. An improvement in the method of performing NMR  
3 imaging with a patient comprising administering to  
4 the patient, an effective amount of a chelate of a  
5 compound of Claim 1, 2, 3, 4, 5, 6, 7 or 8 with a  
6 metal ion having an atomic number of from 21-29, 42,  
7 44 or 58-70.
- 1 45. An improvement in the method for performing NMR  
2 imaging of Claim 44 wherein the metal ion is  
3 selected from the group consisting of chromium(III),  
4 manganese(II), iron(III), iron(II), cobalt(II),  
5 nickel(II), copper(II), praseodymium(III),  
6 neodymium(III), samarium(III), ytterbium(III),  
7 gadolinium(III), terbium(III), dysprosium(III),  
8 holmium(III) and erbium(III).
- 1 46. An improvement in the method for performing NMR  
2 imaging of Claim 44 wherein the chelate of the  
3 compound is a calcium salt.
- 1 47. An improvement in the method for performing NMR  
2 imaging of Claim 46 wherein the molar ratio of  
3 calcium to chelate is from 0.05 to 1.0.

- 1 48. An improvement in the method for performing NMR  
2 imaging of Claim 47 wherein the molar ratio of  
3 calcium to chelate is from 0.1 to 0.5.
- 1 49. An improvement in the method for performing NMR  
2 imaging of Claim 44 wherein the the metal ion is  
3 manganese(II) ion.
- 1 50. An improvement in the method for performing NMR  
2 imaging of Claim 44 wherein the compound is  
3 N,N'-bis-(pyridoxal-5-phosphate)ethylenediamine-  
4 N,N'-diacetic acid, N,N'-bis-(pyridoxl)-  
5 5-phosphate)-trans-1,2-cyclohexyldiamine-N,N'-diaceti  
6 c acid, or a salt thereof.
- 1 51. An improvement in the method for performing NMR  
2 imaging of Claim 44 wherein the metal ion is  
3 manganese(II) and the compound is  
4 N,N'-bis-(pyridoxal-5-phosphate)ethylenediamine-  
5 N,N'-diacetic acid, N,N'-bis-(pyridoxl)-  
6 5-phosphate)-trans-1,2-cyclohexyldiamine-N,N'-diaceti  
7 c acid, or a salt thereof.
- 1 52. An improvement in the method for performing NMR  
2 imaging of Claim 51 wherein the salt is a calcium  
3 salt with a molar ratio of calcium to chelating  
4 compound of from 0.05 to 1.0.
- 1 53. An improvement in the method of performing NMR  
2 imaging of Claim 44 wherein from 0.001 to 5 mmole of  
3 chelate is administered per kg of patient body  
4 weight.
- 1 54. An improvement in the method of performing NMR  
2 imaging of Claim 53 wherein from 0.02 to 0.5 mmole  
3 of chelate is administered per kg of patient body  
4 weight.